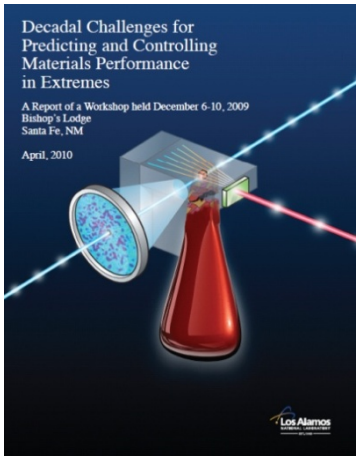
Operated by Los Alamos National Security, LLC,
for the U.S. Department of Energy

LA-UR-11-10856

MaRIE:

(**Ma**tter-**R**adiation **I**nteractions in **E**xtremes)

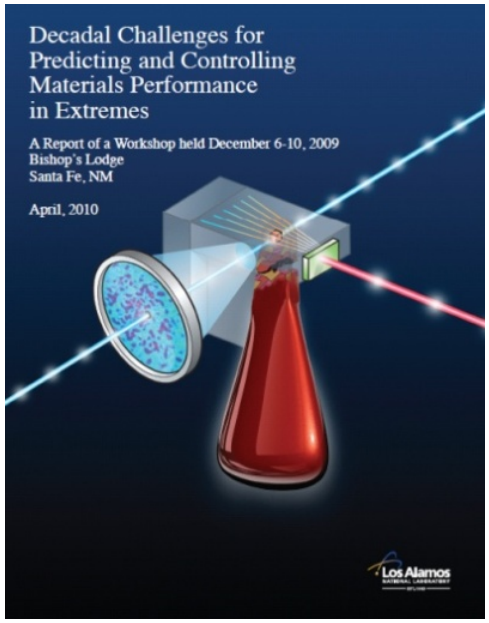
An Experimental Facility Concept Revolutionizing Materials in Extremes



Cris W. Barnes
Los Alamos National Laboratory

Materials research is on the brink of a new era – moving from observation of performance to control of properties

- **The confluence of improved experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible**



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

in extreme environments

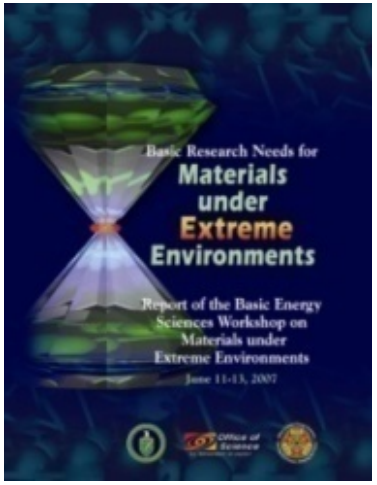
dynamic loading, irradiation

coupled with predictive modeling and simulation

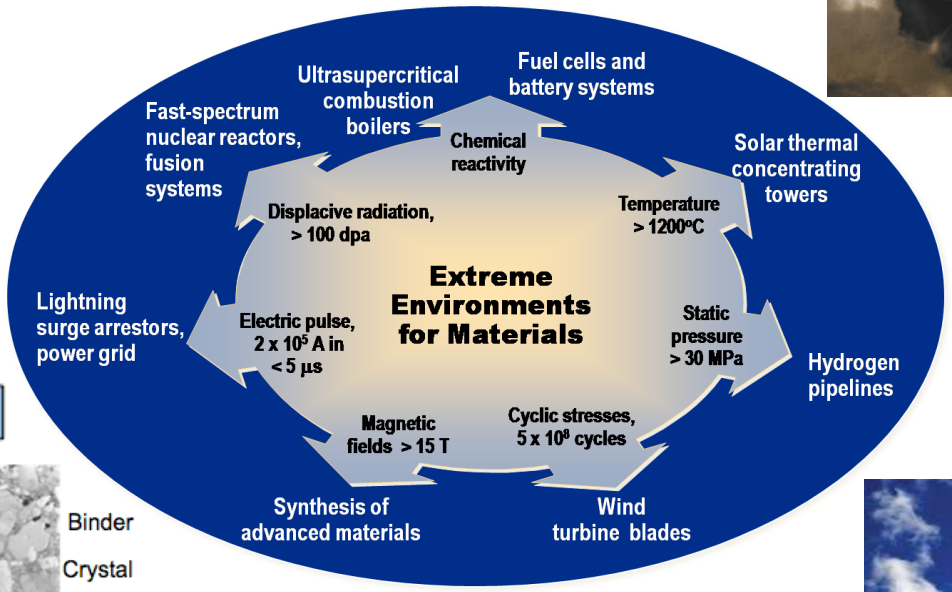
materials design & discovery

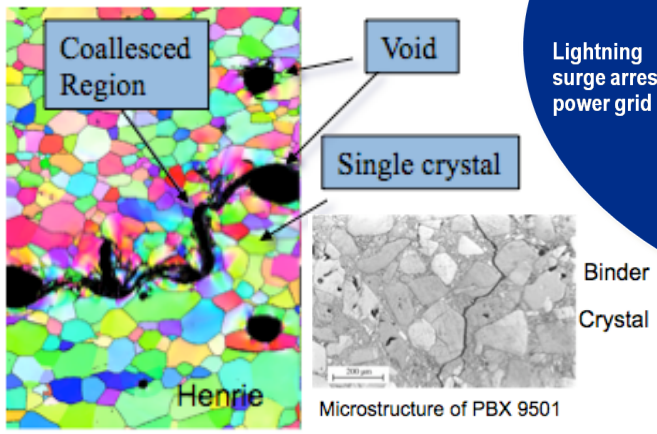
MaRIE builds on unique LANL capabilities to provide the unique experimental tools needed to realize this vision

The needs for materials in extremes are many; the challenge is common: revolutionary advances in controlled functionality

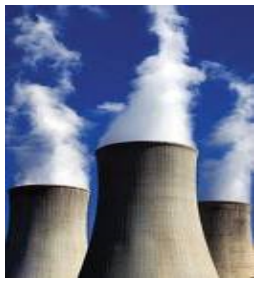


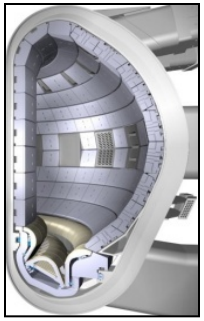
MATERIALS MATTER!!





Microstructure of PBX 9501



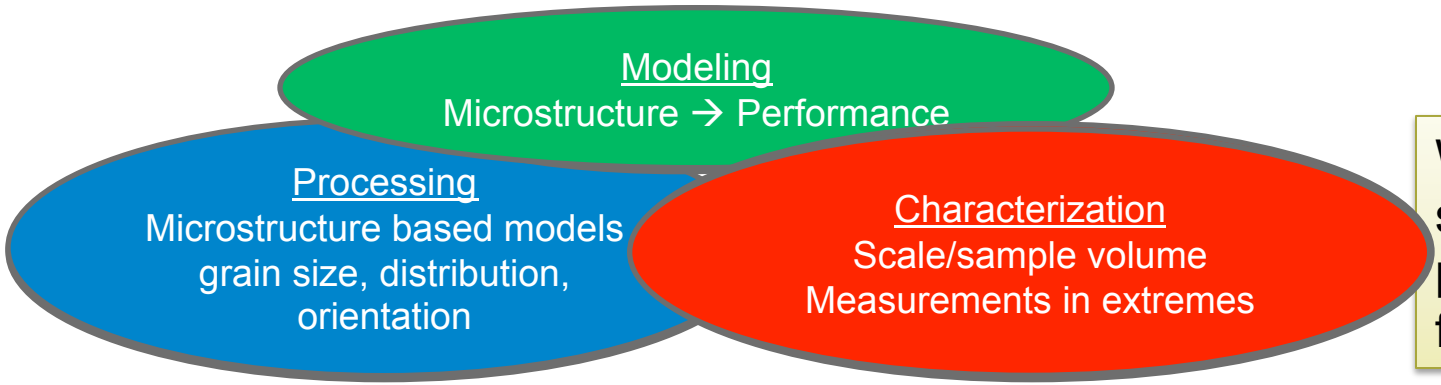


Accelerating complex materials design and discovery requires "integration"

"Physicists perform elegant experiments on crummy samples while materials scientists perform crummy experiments on elegant samples"

-Sig Hecker
Former LANL Director
(materials scientist)

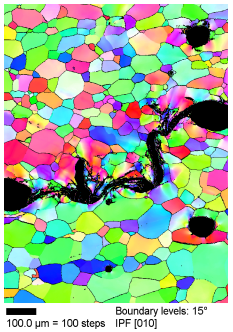
Process Aware Materials Performance



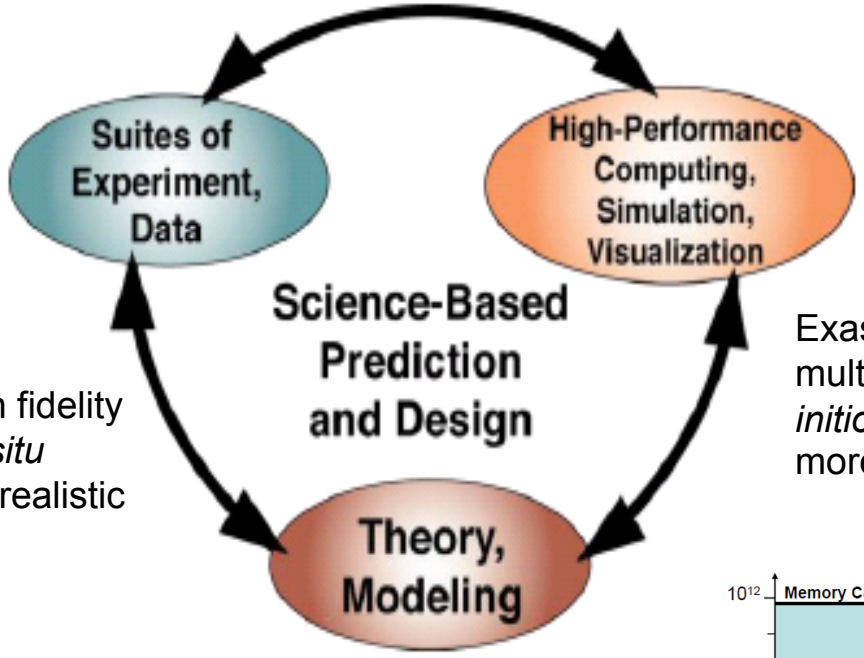
We must move from structure → property paradigm to function → structure

Composition/ Structure ⟷ Theory ⟷ Microstructure/ Properties ⟷ Models ⟷ Devices/ Performance

There is a Decadal Opportunity for the next generation simulation capabilities and experimental tools to enable discovery science at the "micron frontier"

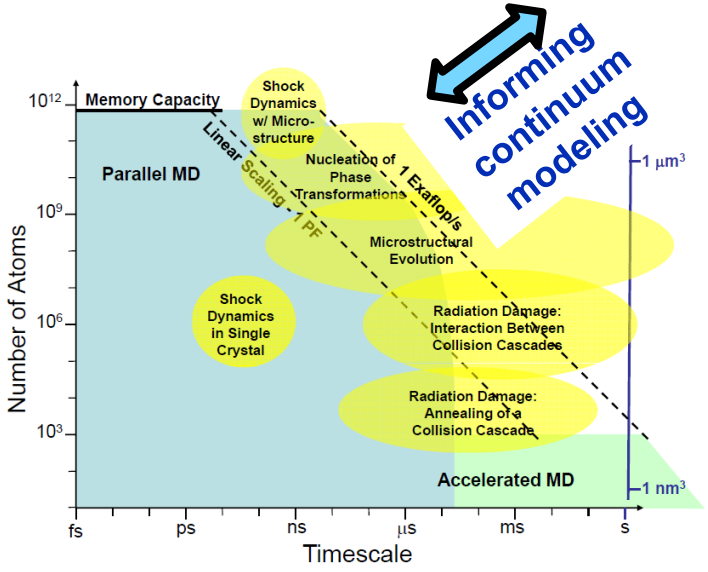


Controlled fabrication, high fidelity characterization, novel *in situ* diagnostics, generation of realistic extreme environments, …



Exascale computing, multi-scale, multi-physics simulation tools, *ab initio* methods applied to larger, more complex materials, …

Multi-scale approaches to connect fundamental scales to bulk properties, defect generation and evolution, …

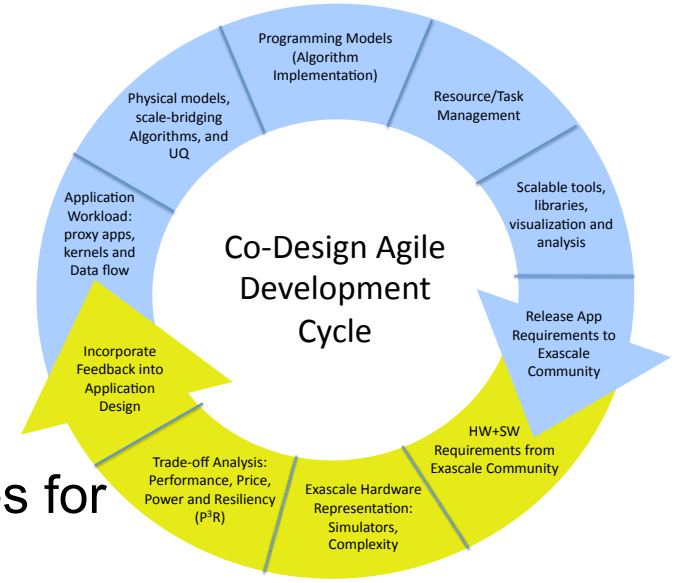


Co-Design is a *process* by which experts in hardware, software, applied mathematics, and domain science work together to enable scientific discovery

- **Exascale computing will transform computational materials science by enabling the pervasive embedding of microscopic behavior into meso- and macroscale materials simulation.**

Exascale Codesign for Materials in Extremes (ExMatEx)

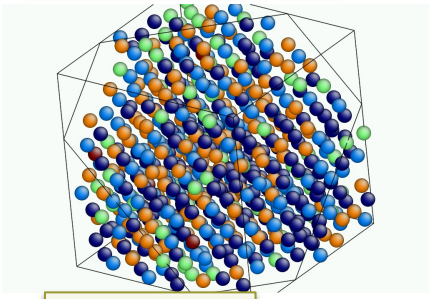
- **ExMatEx will focus effort in 4 areas:**
  - *Scale-bridging algorithms*
  - *Proxy applications*
  - *Hierarchical programming models*
  - *Holistic analysis and optimization*
    - A tightly coupled co-design loop will optimize algorithms and architectures for performance, memory and data movement, power, and resiliency.



Exascale Codesign for Materials in Extremes (ExMatEx)

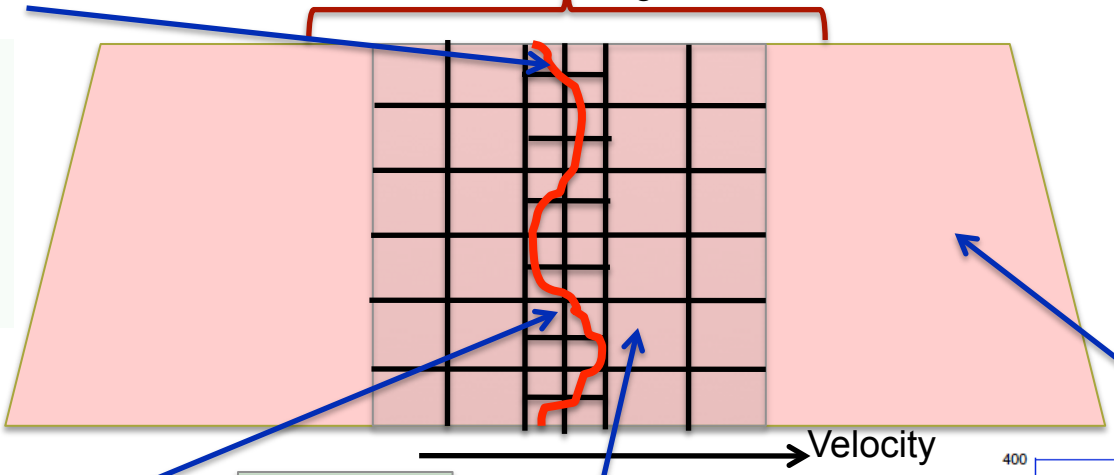
Our Strategy: an Uncertainty Quantification (UQ) approach to Adaptive Physics Refinement

dt ≈ 0.001-.01 ps



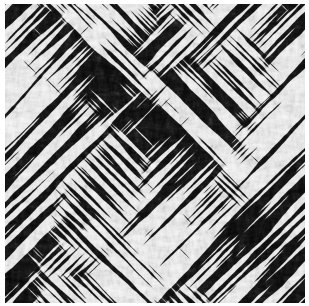
Atomistics

Moving refinement window



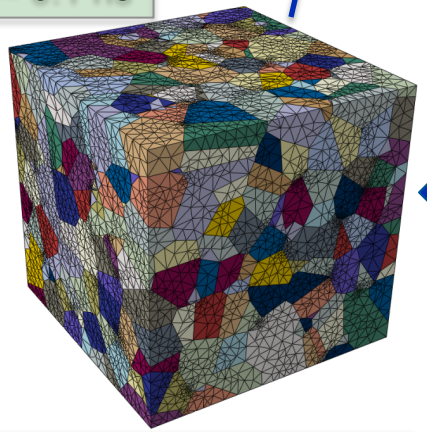
dt ≈ 2 ns

dt ≈ 0.01-.1 ns

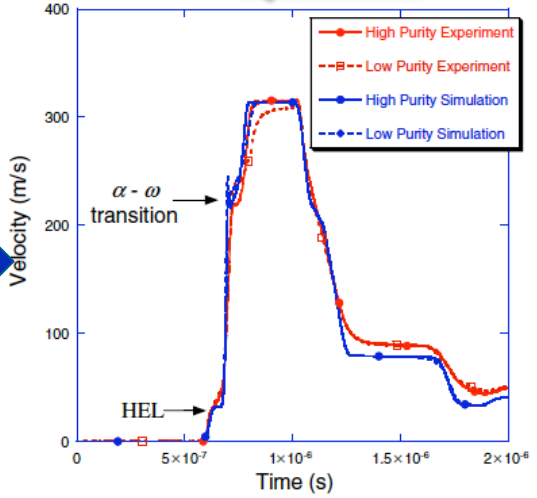


Single crystal (1)

dt ≈ 0.1 ns



Polycrystal (≈ 8X8X8)



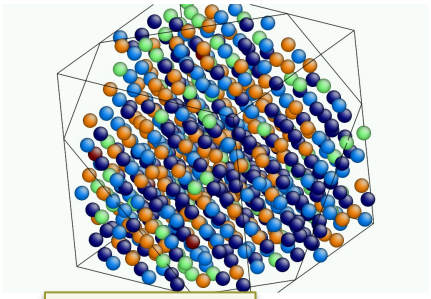
Continuum (≈> 8)

NATIONAL LABORATORY
EST.1943

Coarse-scale simulations spawn sub-scale direct simulations as needed.

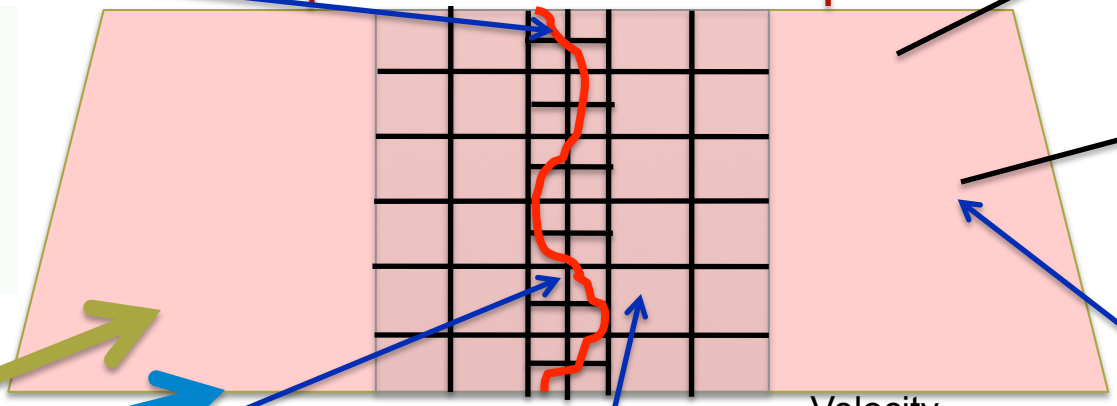
Our Strategy: an Uncertainty Quantification (UQ) approach to Adaptive Physics Refinement

dt ≈ 0.001-.01 ps

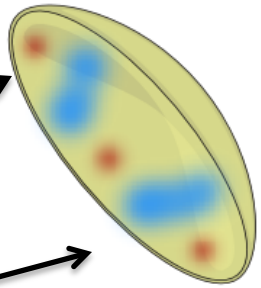


Atomistics

Moving refinement window



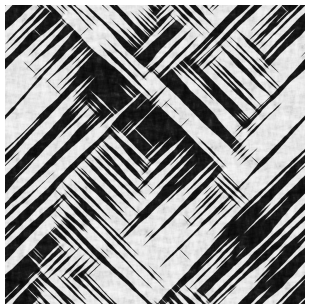
Velocity



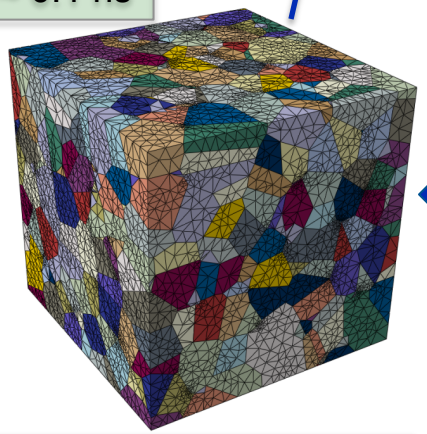
dt ≈ 2 ns

dt ≈ 0.1 ns

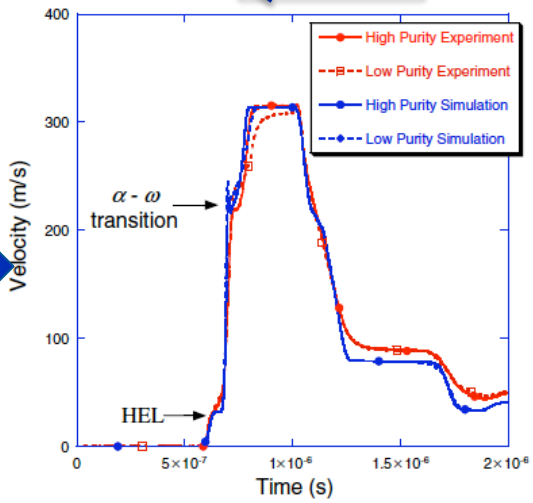
dt ≈ 0.01-.1 ns



Single crystal (1)



Polycrystal (≈ 8X8X8)



Continuum (≈> 8)

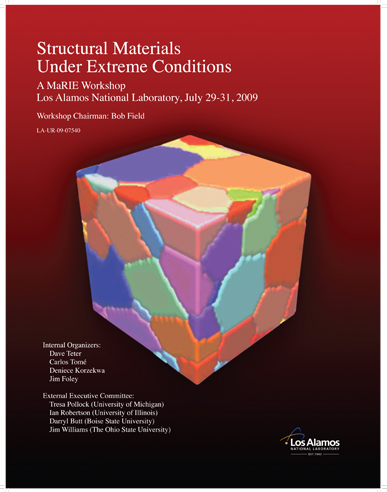
Coarse-scale simulations spawn sub-scale direct simulations as needed.

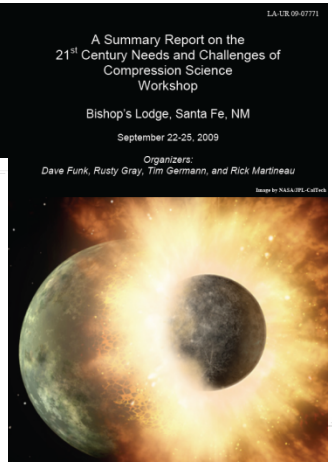
Science-driven Requirements Lead to Integrated Facility Needs Fulfilled by MaRIE

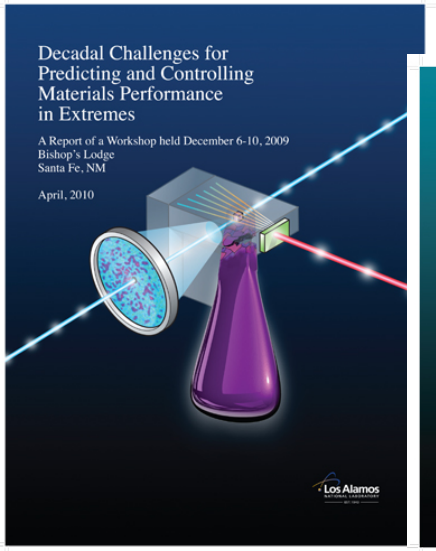
MaRIE will address problems central to Department of Energy missions in energy, science, and security

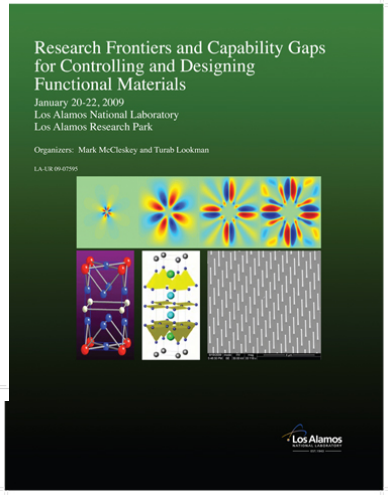
- What are the consequences of materials failure for weapons performance?
- How do we accelerate the certification of materials to enable a nuclear renaissance?
- Can we predict and prevent materials damage?
- Can we discover by design materials to perform in unprecedented irradiation extremes?
- How do we predict and control microstructure for designed materials performance?
- Can we design and synthesize new materials with controlled functionality?

Community-based workshops have helped to define the decadal challenges for predicting and controlling materials performance in extremes



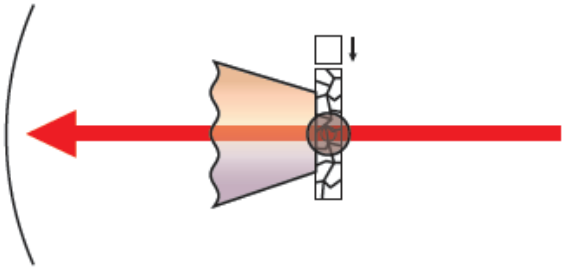


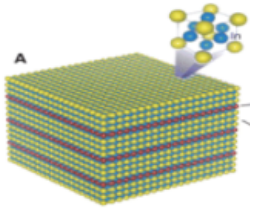


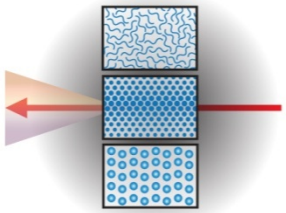


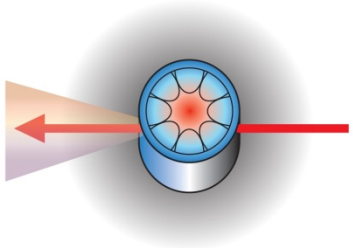
http://marie.lanl.gov/source/projects/marie/workshops.shtml

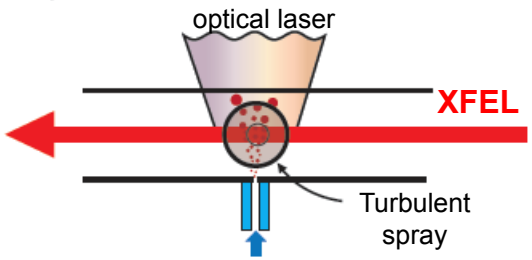
First experiment teams include ~170 scientists from ~ 60 institutions in 10 countries

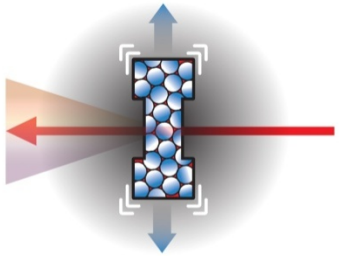


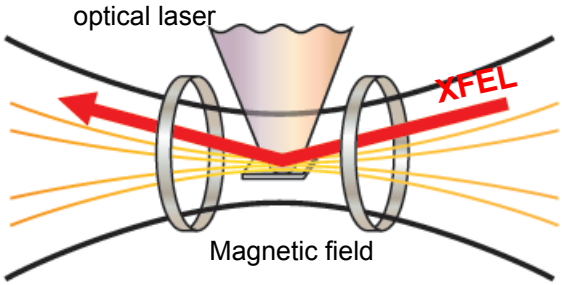


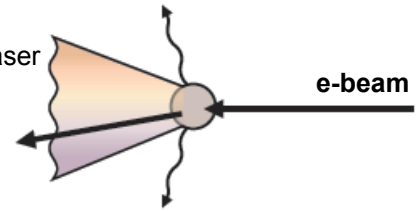


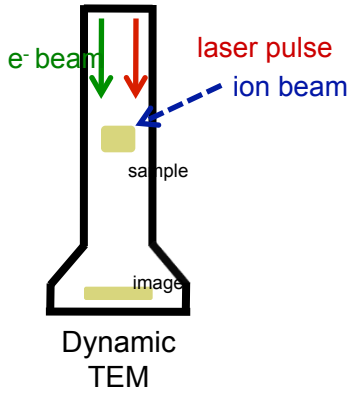


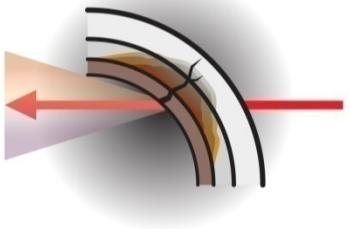






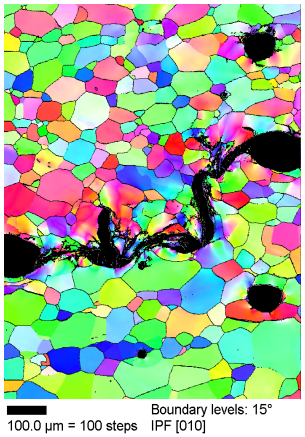




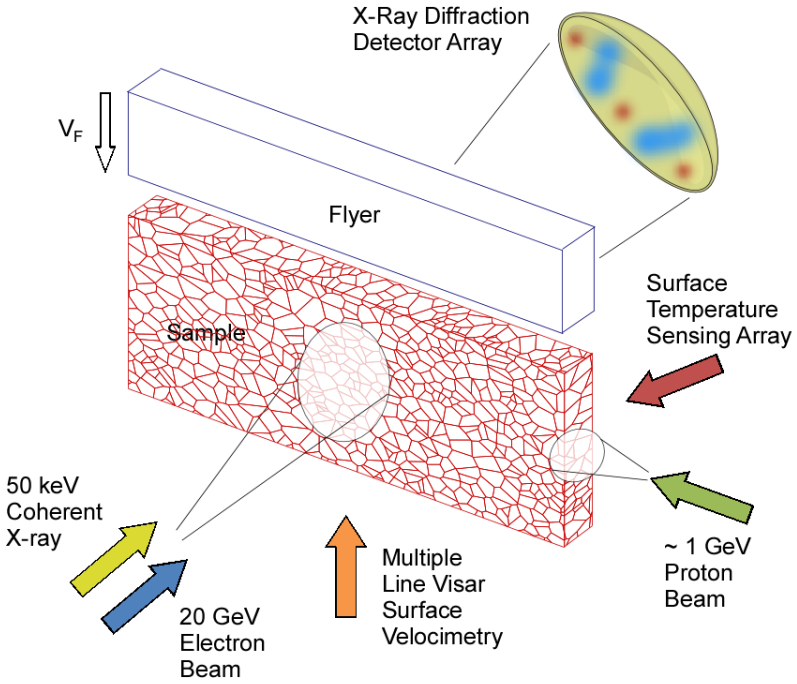


We're laying the foundation for a robust MaRIE user community

Understanding the role of microstructure-based heterogeneity evolution in material damage



The goal :- Predict dynamic microstructure and damage evolution



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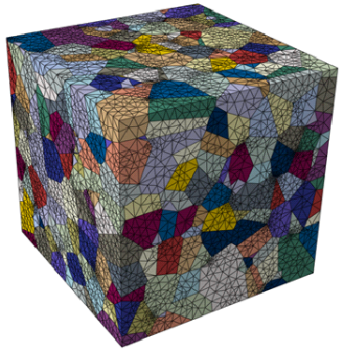


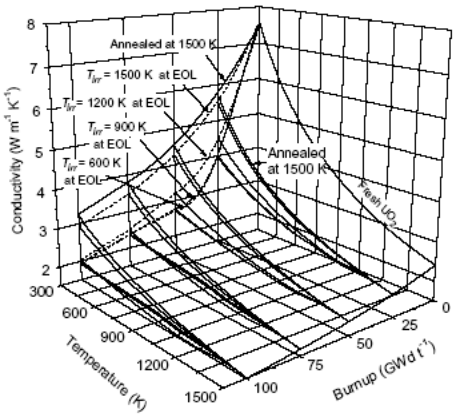
Meso-Scale Theory and Simulation

The first experiment :- Multiple, simultaneous dynamic in situ diagnostics with resolution at the scale of nucleation sites (< 1 µm; ps – ns)

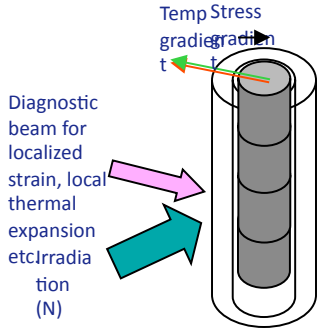
The model :- Accurate sub-grain models of microstructure evolution coupled to molecular dynamics

Team includes: Curt Bronkhorst et al. (LANL, UK AWE, BYU, CalTech, Ohio State, …)

Determining spatially-resolved thermophysical properties in prototype nuclear fuel geometries

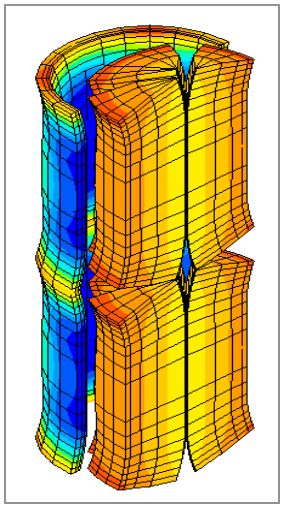


Predicted and measured UO2 thermal conductivity



Goal :- Spatially resolved predictions and measurements of engineering performance of prototype fuel pin geometries as a function of power, burnup and time

Experiment :- MaRIE will use photons, (electrons & neutrons) to make unique measurements of phase, strain, microstructure, porosity & temperature distributions on engineering scale samples in & out of a radiation environment

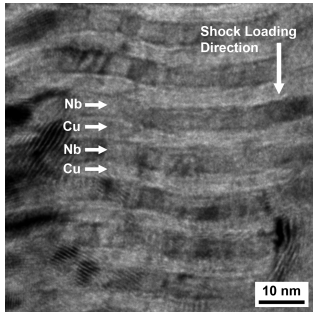


(PLEIADES code, CEA, France)

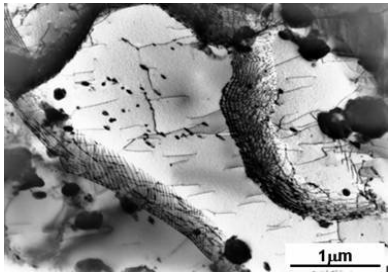
Model :- Stress/ Temperature Field in a Fuel Element consisting of two ceramic pellets and metallic clad.

Team includes: Marius Stan et al. (LANL, ANL, Wisconsin, INL, CEA …)

Understanding the role of interfaces in strain evolution

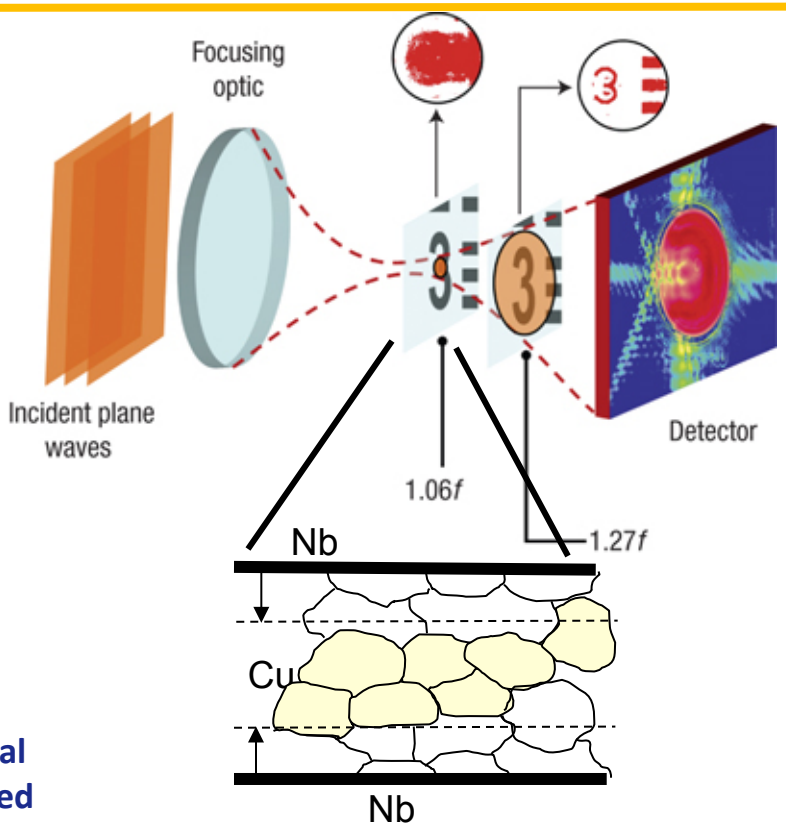


Nano laminates

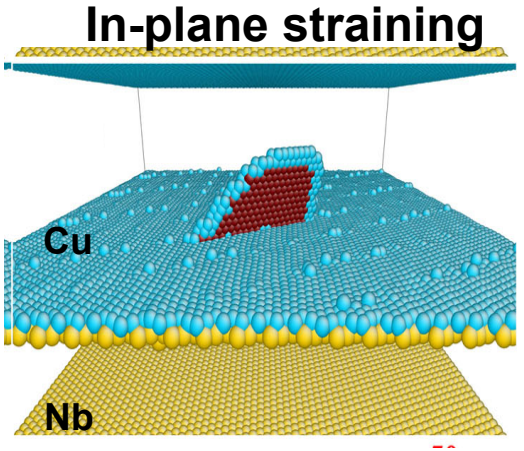


ODS steel

The goal : Predict interfacial microstructure for increased strength and irradiation resistance



The first experiment : 3-D movies of dislocation dynamics in materials at buried interfaces, micron field of view with focusing at nm resolution



The model :Advanced M²S with micron scale, multigranular predictions

Team includes: Nate Mara et al. (LANL, ANL, CMU…)

MaRIE photon needs can be met by an XFEL that is technically feasible and affordable and provides unique scattering and imaging capabilities to bridge the micron gap in extreme environments

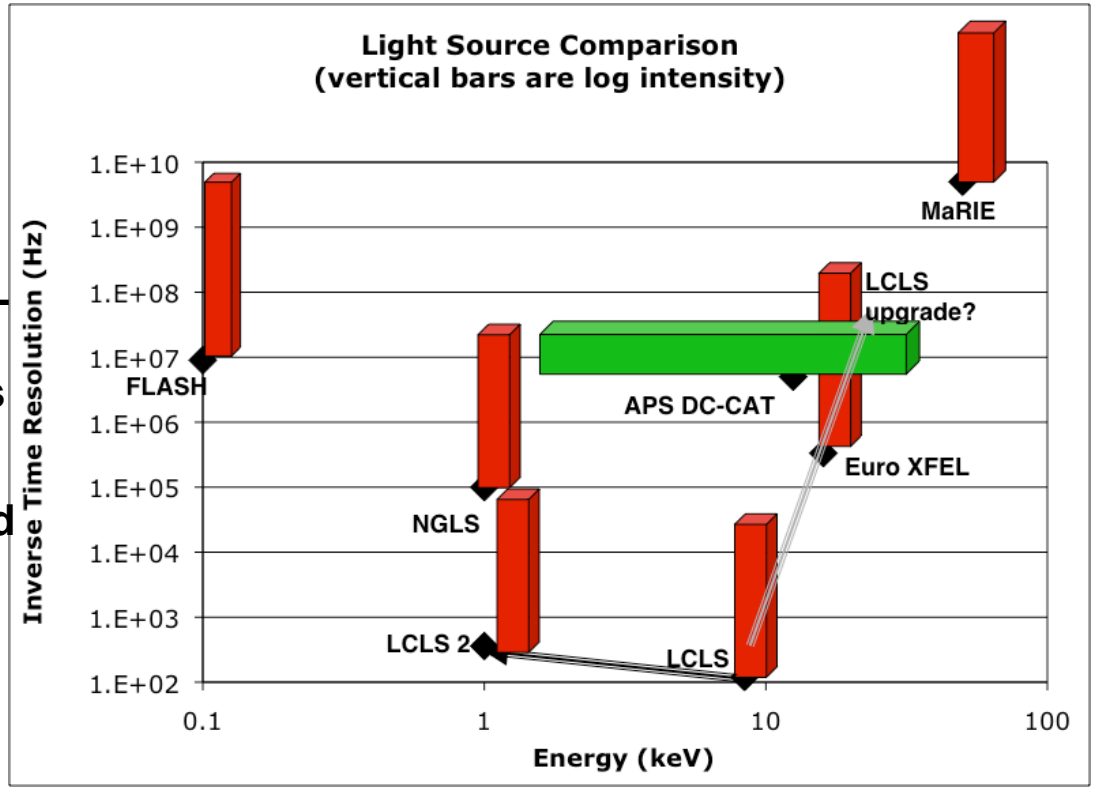
Light Sources are differentiated by:

- Energy
- Peak Brightness
- Average Brightness
- Hutches (beam lines)

MaRIE is a very-hard x-ray (50-keV) FEL (high peak) with several (~5) hutches but low average brightness

It is aimed at mesoscale material dynamics and radiation damage and *in-situ* measurements of multi-granular stochastic samples whose performance is determined by rare events

A high-energy-photon (50-115 keV) XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation



Science-driven Requirements Lead to Integrated Facility Needs Fulfilled by MaRIE

User Driven Science → Materiel Needs → **Functional Requirements** → Alternatives Analyses → **Performance Gaps** → Preferred Alternative & Roadmap → **Facility Concept**

Dynamic Extremes
- Microstructure Evolution
- Stochastic Explosive Microstructure & Detonation
- Fluid/Mineral Interactions in
- 3-D Measurements of Turbulent

Radiation Extremes
- Irradiation Stability of Structural Nanocomposites
- Fission Gas Bubble & Swelling in UO_2 Nuclear Fuel
- Mechanical Testing of Structural Mateials in Fusion/Fission Environ.
- Measurements of Temperature, Microstructure & Thermal Transport
- Rad Damage in Passive Oxide Films & its Influence on Corrosion

Control of Complex Materials & Processes
- Understanding Emergent Phenomena in Complex Materials
- Developing Practical Superconductors by Design

Energy Conversion & Storage
- Achieving Practical High-Density Energy Storage Through New Support/Catalyst Electrode Systems
- Solar Energy Conversion w/ Fun-ctionally Integrated Nanostructures

Process-Aware Materials Performance
- Nanostructured Ferritic Alloys
- Exploring Separate Effects in Pu

Environments
- Dynamic pressure <200 GPa
- Strain rate = 10^{1}–10^{7} s^{-1}
- Temperature = 77–2000 K
- High Explosives < 30 g
- Pu isotope samples < 3 mm thick
- Irradiation rate < 35 dpa/fpy
- He(appm)/dpa ratios: 0.1-1, 9-13
- Irrad Volume: 0.5 l @ >14 dpa/yr

Measurements
- Scattering
  - Defects: 1 nm res over 10 um
  - Stress: 1-2 um res over 100 mm
  - Lattice Strain: 10 nm res in 3D
- Density Imaging
  - 0.1-1 nm, <1-ps res over 10 μm
  - 10 nm, <1-ps over 50 μm
  - 0.1-1 um, < 0.3 ns over 0.1-1 mm
- Spectroscopic
  - 3D chemistry mapping w/ 1μm res
- Themo-Physical Measurements
  - Temperature: 1 μm res
  - Thermal Conductivity w/ 1 mW/m-K res

Synthesis with Characterization
- Organic, inorganic, biomaterials incl nanomaterials, HE & actinides
- Thin films with buried interface characterization

50 keV coherent x-ray source with 10^{11} photons per macropulse focused to 1-200 μm

Dynamic charged particle imaging with 20-GeV electrons

Tunable ultrashort x-ray source for excitation: 5-35 keV, 100 fs, focused to 10 nm

Ultra short pulse lasers for spectroscopy: THz (2 meV) to VUV (6 eV)

MW fast neutron source with $2x10^{15}$ n/cm2-s and >4000 h/yr operation with < 10 beam trips per day over 1 min

Crystal growth with control of impurities & defects during and after fab

Deposition Lab w/CVD, PVD, evaporation, ion beams

Nanofabricaiton Lab w/ lithography, dry & wet etch, thermal processing

Characterization Lab w/ SEM, FE-SEM, AFM, SALVE, ion beams

Data Visualization Lab w/ 1MB-10TB available per expt.

MaRIE builds upon existing $B investments at LANSCE with the addition of the:

- Electron Linac with XFEL Systems
- Multiprobe Diagnostic Hall
- Fission-Fusion Materials Facility
- Making, Measuring, & Modeling Material Facility

At LANSCE today, a flexible 1 MW, 800 MeV proton accelerator drives several user facilities

Unique, highly-flexible beam delivery to multiple facilities 6 mo/yr @ 24/7 with ~ 1200 user visits

Lujan Center

- *Materials science and condensed matter research*
- *Bio-science*
- *Nuclear physics*
- *A National BES user facility*

WNR

- *Nuclear physics*
- *Semiconductor irradiation*

Ultra-cold Neutron Facility

- *Fundamental nuclear physics*

Proton Radiography

- *HE science, dynamic materials science, hydrodynamics*

Isotope Production Facility

- *Nuclear medicine*
- *Research isotope production*

MaRIE builds on the LANSCE facility to provide unique co-located experimental tools to realize transformational advances in materials performance in extremes

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

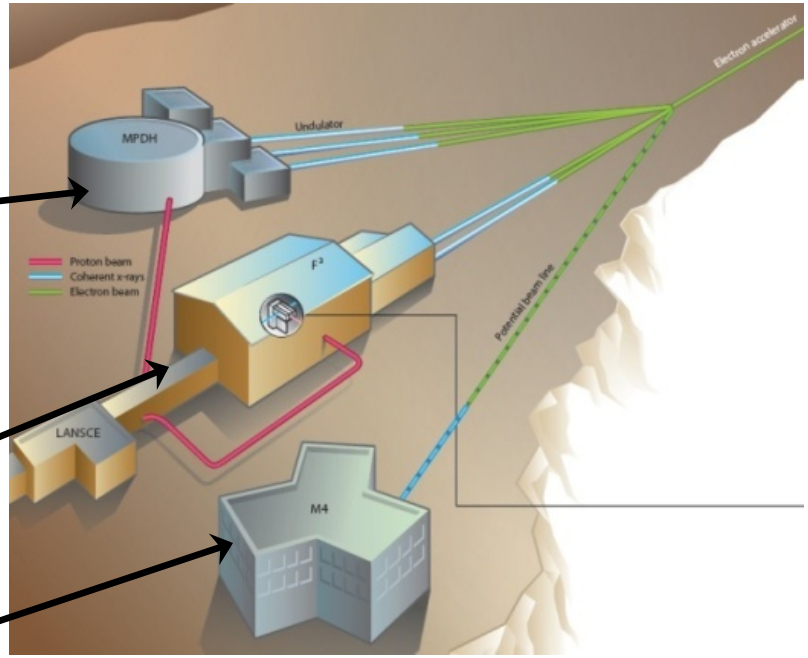
(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(**M4**: Making, Measuring & Modeling Materials Facility)

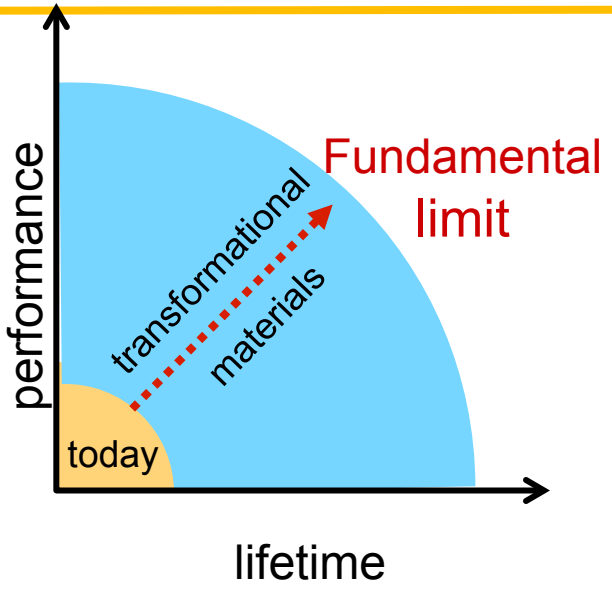


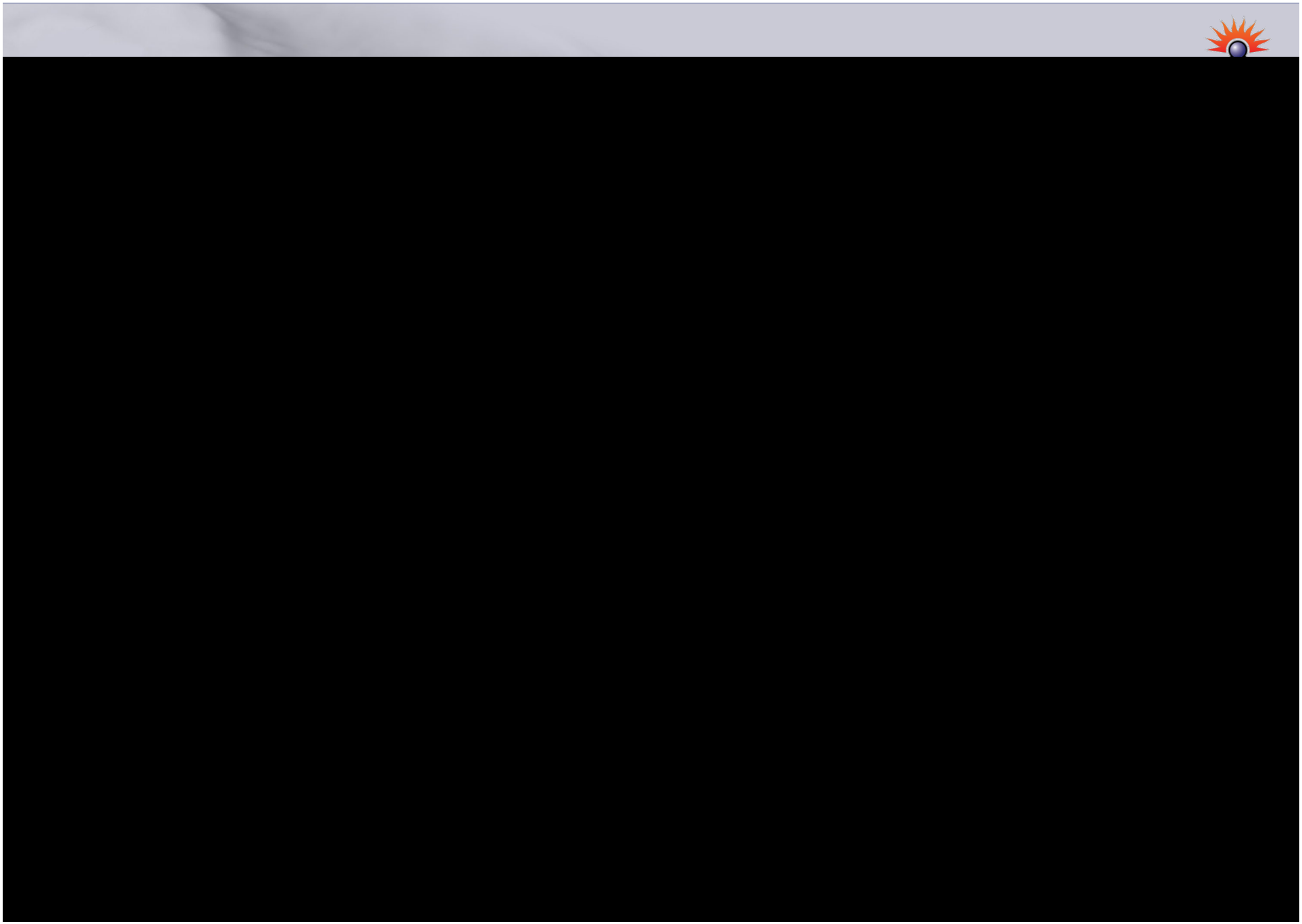
Unique very hard x-ray XFEL
Unique simultaneous photon-proton imaging measurements
Unique spallation neutron-based irradiation capability
Unique in-situ, transient radiation damage measurements
Unique materials design and discovery capability

MaRIE will provide unprecedented international user resources

MaRIE will be the first capability with unique co-located tools necessary to revolutionize materials in extremes

- **Materials research is on the brink of a new era – moving from observation of performance to control of properties**
- **There is a Decadal Opportunity for the next generation simulation capabilities and experimental tools to enable discovery science at the "micron frontier"**
- **Science-driven requirements lead to integrated facility needs fulfilled by MaRIE**





Thank you for your attention!